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Editorial

Photon and Particle Impact Spectroscopy and Dynamics of Atoms, Molecules and Clusters

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1. Introduction

Atomic, molecular, and optical (AMO) physics is a vastly important sub-discipline. It provides insights into the fundamental nature of matter, drives technological innovation, and contributes to various scientific and applied fields across disciplines. Since the early days of quantum mechanics, AMO physics has allowed for the exploration of the fundamental processes that govern the behavior of atoms and molecules. This includes understanding the structure of atoms, the nature of chemical bonds, and the dynamics of AMO interactions. Many advanced processes were discovered and controlled, such as developments in lasers, spectroscopy, and quantum optics. These have had profound impacts on technology, ranging from medical imaging to communication systems [1]. AMO physics plays a vital role in the emerging field of quantum information science. Research in this field aims to harness the principles of quantum mechanics to manipulate and control quantum states to develop powerful quantum computers and communication systems [2]. Techniques developed in AMO physics are used for highly precise measurements, such as atomic clocks and global positioning systems [3]. AMO physics provided the ground, knowledge, and original field of applications in creating ultrashort pulses of light that can now measure the rapid processes in which electrons move or change energy in materials—a technology that was the topic of the 2023 Nobel Prize in Physics [4]. Advancing into materials science, AMO physics contributes to the development of new materials with specific properties, impacting areas, such as electronics, nanotechnology, and energy storage. Techniques from AMO physics are vital for medical diagnostics [5] that include advances in laser technology finding applications in medical treatments and surgeries. AMO physics contributes to the understanding of the universe, including the behavior of matter under extreme conditions found in stars and other astrophysical environments [6]. Coming back to the basics, AMO physics is still a powerhouse in addressing fundamental questions about the nature of matter and the universe. For example, studying ultracold atoms [7], quantum gases, and interactions involving antimatters [8] allows us to explore exotic states of matter and test the limits of our understanding of quantum mechanics and fundamental forces. In all the above, computational AMO physics offers essential machinery. It complements experiments, transforms the hypothesis to mathematical expectations, predicts and interprets measurements, forecasts new materials before synthesis, and contributes to the understanding of complex physical phenomena. Thus, computational AMO physics tackles the challenges posed by the complex nature of quantum systems, providing valuable insights and facilitating advancements in technological domains.

Therefore, research and development in AMO physics are vastly active and organically developing to invent many sub-fields of interest. The current Special Issue (SI), entitled *Photon and Particle Impact Spectroscopy and Dynamics of Atoms, Molecules, and Clusters*, is a modest but valuable effort to publish some novel research by renowned AMO research groups and scientists. A total of thirteen articles encompasses a collection

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of research findings in the interaction of charged particles and lights with varieties of AMO systems.

A Rundown of Articles

Proton: Two articles are published reporting measurements of the energetic proton impact fragmentation of molecules. The one by *Vinitha* et al. (contribution 1). measures multi-fragmentation of highly charged azulene and naphthalene ions produced in 50–150 keV proton collisions via the multi-hit time-of-flight experimental technique. Such spectroscopic results serve as crucial aspects in the diagnosis of hostile celestial regions, where polycyclic aromatic hydrocarbons are abundant and under constant bombardment by protons in the stellar wind. The other article, by *Duley and Kelkar* (contribution 7), considers the dissociation dynamics of carbon dioxide molecular ions impacted by 1 keV protons measured with a recoil-ion momentum spectrometer. Broadly speaking, such studies are important in plasma physics, hydrocarbon chemistry, as well as in modelling interstellar media.

Electron: Two articles report on theoretical electron-impact studies—both on fundamental interaction grounds. The one by *Msezane and Felfli* (contribution 10) studies the low-energy electron attachment process using a quantum mechanical effect of Ramsauer–Townsend minima based on the Regge pole analysis. This addresses the fundamental question of the origin and character of the electron affinity for large atoms: does the electron affinity of these systems characterize from the ground, metastable or excited states of their negative ions? The other study by Harris (contribution 6) examines a novel mechanism of selectively sculpted electron beams to collide with the helium atom in order to explore effects of the coherence length of the projectile wave packets. This study may lead to a new direction of measurements involving collisions with twisted beams of charged particles.

Photon: There are several articles that investigate the interactions of electromagnetic radiation with AMO systems. One article by *Hosea* et al. (contribution 2) theoretically explores the effect of the interference between the electric dipole and quadrupole order of coupling of the photon with a sodium atom for its valence photoionization. This is carried out near a spectrally sensitive feature as a function of energy called the Cooper minimum. The study paves a track to access even higher multipole effects. The other study, by *Shaik* et al. (contribution 3), focuses on the single-photon dipole photoionization of three magic-number sodium clusters in a framework of density functional theory to explore fascinating spectral features. The ultrafast timing of the photoionization process in attoseconds has been investigated on a fundamental theoretical track of Eisenbud–Wigner–Smith (EWS) in two papers. The one by *Grafstrom* and *Landman* (contribution 5) uses the relativistic random-phase approximation to calculate the time delay from outer subshells of various isoelectronic noble gas neutrals and anions. The other paper, by *Baral* et al. (contribution 8), applies the same theory to examine the modification in the EWS delay for the electron ejection from noble gas atoms within an optical dipole trap, a possible prototype for the qubit in quantum computing. A pair of theory articles have been published on research involving interactions with strong (multi-photon) radiation fields as well. In one of these, a study by *Simonovic* et al. (contribution 11) reports Rabi oscillation dynamics driven by intense, short, resonant laser pulses and invalidates a hypothesis about the origin of the multiple-peak pattern in the photoelectron energy distribution. The other study by *Schimmoller* et al. (contribution 9) performs simulations in the quantum trajectory Monte Carlo method and compares with experiments for a neutral diatomic molecule to demonstrate that the molecular ionization site in the strong-field spectra is insensitive to the pulse's carrier envelop phase.

Plasma: The research by *Biswas* et al. (contribution 4) utilizes a powerful relativistic coupled-cluster theory to study the plasma-field-induced structures and transitions of some high-charge cations of astrophysical relevance. It is expected that the results can be applied for celestial or laboratory plasma diagnostics.

Last but not at all least, we would like to mention two opinion articles published in this SI from two experienced and versatile researchers in AMO fields. The article by *Manson* (contribution 12) discusses the critical implications of an otherwise small force, the spin–orbit force. In fact, the importance of spin–orbit forces extends across branches of physics, from understanding the behavior of electrons in atoms to the structure of atomic nuclei and the properties of exotic matter. The inclusion of spin–orbit effects is crucial for accurate modeling and predicting the behavior of particles and systems in a wide range of physical scenarios. The other opinion article, by *Connerade* (contribution 13), delves into examples of contemporary physics questions to argue that atomic physics remains at the epicenter to test fundamental principles of physics, which are still inadequately understood. We re-quote Richard Feynman from this article. "When asked: should Armageddon occur, is there a simple, most important idea to preserve as a testament to human knowledge? The answer he suggested is the atomic hypothesis".

2. Future Research Prospects

We take this opportunity to comment on some future research roadmaps in AMO science that may emanate from the current landscape. The ongoing drive of strong pulsed-laser field research will increasingly empower the control, imaging, and manipulation of electron and ion-core dynamics on ultrafast timescales [9,10]. Such ultrafast spectroscopy and imaging, even for weak laser fields where the pristine electronic phenomena can be better captured, will have applications in studying chemical reactions, biological processes, and material properties [11,12]. This can further generate a focus direction of accessing the dephasing dynamics of plasmon resonances to enrich quantum plasmonic applications [13]. Future research on quantum information science may focus on the creation and manipulation of more robust and scalable qubits. This can explore new quantum algorithms, addressing challenges in quantum error correction. Likewise, AMO research on quantum optics may involve developing methods for quantum state engineering, communication, and sensing using techniques, like cavity quantum electrodynamics and laser cooling [14]. Continued exploration of ultracold quantum gases, such as Bose–Einstein condensates for quantum many-body physics and phase transitions, may investigate novel applications of ultracold atoms in precision measurements and quantum simulation [15,16]. Another particularly interesting direction is the integration of superconducting circuits with ion traps and AMO systems creating hybrid quantum systems [17]. This can lead to enhanced coherence times and improved quantum gates for applications in quantum technologies. Finally, investigating the interaction of AMO systems with emerging materials and interfaces [18] may explore novel phenomena and applications in areas like nanotechnology and condensed matter physics.

3. Conclusions

The original dream for the driving objective of this SI was that submissions should present novel effects, mechanisms, and phenomena in the energy response (spectroscopy) and the time evolution (dynamics) of excited target systems, highlighting new experimental techniques and powerful theoretical/computational methods and instigating novel questions to motivate future research and collaboration. On the other hand, today's AMO physics research dissemination is motivated by a dual commitment to featuring fundamental discoveries and to utilizing some of that knowledge for future technological applications. To that fantastically lofty goal, the current SI serves as a small but important leap forward.

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List of Contributions

1. Vinitha, M.V.; Bhatt, P.; Safvan, C.P.; Vig, S.; Kadhane, U.R. Fragmentation of Multiply Charged C10H8 Isomers Produced in keV Range Proton Collision. *Atoms* **2023**, *11*, 138. https://doi.org/10.3390/atoms11110138.
2. Hosea, N.M.; Jose, J.; Varma, H.R.; Deshmukh, P.C.; Manson, S.T. Quadrupole Effects in the Photoionisation of Sodium 3s in the Vicinity of the Dipole Cooper Minimum. *Atoms* **2023**, *11*, 125. https://doi.org/10.3390/atoms11100125.
3. Shaik, R.; Varma, H.R.; Chakraborty, H.S. Density Functional Treatment of Photoionization of Sodium Clusters: Effects of Cluster Size and Exchange–Correlation Framework. *Atoms* **2023**, *11*, 114. https://doi.org/10.3390/atoms11080114.
4. Biswas, S.; Bhowmik, A.; Das, A.; Pal, R.R.; Majumder, S. Transitional Strength under Plasma: Precise Estimations of Astrophysically Relevant Electromagnetic Transitions of Ar^{7+}, Kr^{7+}, Xe^{7+}, and Rn^{7+} under Plasma Atmosphere. *Atoms* **2023**, *11*, 87. https://doi.org/10.3390/atoms11060087.
5. Grafstrom, B.; Landsman, A.S. Attosecond Time Delay Trends across the Isoelectronic Noble Gas Sequence. *Atoms* **2023**, *11*, 84. https://doi.org/10.3390/atoms11050084.
6. Harris, A.L. Projectile Coherence Effects in Twisted Electron Ionization of Helium. *Atoms* **2023**, *11*, 79. https://doi.org/10.3390/atoms11050079.
7. Duley, A.; Kelkar, A.H. Fragmentation Dynamics of COq+2 (q = 2, 3) in Collisions with 1 MeV Proton. *Atoms* **2023**, *11*, 75. https://doi.org/10.3390/atoms11050075.
8. Baral, S.; Easwaran, R.K.; Jose, J.; Ganesan, A.; Deshmukh, P.C. Temporal Response of Atoms Trapped in an Optical Dipole Trap: A Primer on Quantum Computing Speed. *Atoms* **2023**, *11*, 72. https://doi.org/10.3390/atoms11040072.
9. Schimmoller, A.; Pasquinilli, H.; Landsman, A.S. Does Carrier Envelope Phase Affect the Ionization Site in a Neutral Diatomic Molecule? *Atoms* **2023**, *11*, 67. https://doi.org/10.3390/atoms11040067.
10. Msezane, A.Z.; Felfli, Z. Rigorous Negative Ion Binding Energies in Low-Energy Electron Elastic Collisions with Heavy Multi-Electron Atoms and Fullerene Molecules: Validation of Electron Affinities. *Atoms* **2023**, *11*, 47. https://doi.org/10.3390/atoms11030047.
11. Simonović, N.S.; Popović, D.B.; Bunjac, A. Manifestations of Rabi Dynamics in the Photoelectron Energy Spectra at Resonant Two-Photon Ionization of Atom by Intense Short Laser Pulses. *Atoms* **2023**, *11*, 20. https://doi.org/10.3390/atoms11020020.
12. Manson, S.T. The Spin-Orbit Interaction: A Small Force with Large Implications. *Atoms* **2023**, *11*, 90. https://doi.org/10.3390/atoms11060090.
13. Connerade, J.-P. The Atom at the Heart of Physics. *Atoms* **2023**, *11*, 32. https://doi.org/10.3390/atoms11020032.

References

1. National Research Council. *Atoms, Molecules, and Light: AMO Science Enabling the Future*; The National Academies Press: Washington, DC, USA, 2002. [CrossRef]
2. Saffman, M. Quantum computing with atomic qubits and Rydberg interactions: Progress and challenges. *J. Phys. B At. Mol. Opt. Phys.* **2016**, *49*, 20200. [CrossRef]
3. Ludlow, A.D.; Boyd, M.M.; Ye, J.; Peik, E.; Schmidt, P. O. Optical atomic clocks. *Rev. Mod. Phys.* **2015**, *87*, 637. [CrossRef]
4. The Nobel Prize in Physics 2023. Available online: https://www.nobelprize.org/prizes/physics/2023/press-release/ (accessed on 28 November 2023).
5. Weber, S.; Wu, Y.; Wang, J. Recent progress in atomic and molecular physics for controlled fusion and astrophysics. *Matter Radiat. Extremes* **2021**, *6*, 023002. [CrossRef]
6. Higashi, Y.; Matsumoto, K.; Saitoh, H.; Shiro, A.; Ma, Y.; Laird, M. Iodine containing porous organosilica nanoparticles trigger tumor spheroids destruction upon monochromatic X-ray irradiation: DNA breaks and K-edge energy X-ray. *Sci. Rep.* **2021**, *11*, 14192. [CrossRef] [PubMed]
7. Brierley, R.; Li, Y.; Benini, L. Ultracold quantum technologies. *Nat. Phys.* **2021**, *17*, 1293. [CrossRef]
8. Adkinsa, G.S.; Cassidyb, D.B.; Pérez-Ríosc, J. Precision spectroscopy of positronium: Testing bound-state QED theory and the search for physics beyond the Standard Model. *Phys. Rep.* **2022**, *975*, 1–61. [CrossRef]
9. Tóth, A.; Csehi, A. Strong-field control by reverse engineering. *Phys. Rev. A* **2021**, *104*, 063102. [CrossRef]

10. Young, L.; Ueda, K.; Gühr, M.; Bucksbaum, P.H.; Simon, M.; Mukamel, S. Roadmap of ultrafast X-ray atomic and molecular physics. *J. Phys. B At. Mol. Opt. Phys.* **2018**, *51*, 032003. [CrossRef]
11. Maiuri, M.; Garavelli, M.; Cerullo, G. Ultrafast Spectroscopy: State of the Art and Open Challenges. *J. Am. Chem. Soc.* **2020**, *142*, 3–15. [CrossRef] [PubMed]
12. Hutchison, C.D.M.; Baxter, J.M.; Fitzpatrick, A.; Dorlhiac, G.; Fadini, A.; Perrett, S. Optical control of ultrafast structural dynamics in a fluorescent protein. *Nat. Chem.* **2023**, *15*, 1607–1615. [CrossRef] [PubMed]
13. Biswas, S.; Trabattoni, A.; Rupp, P.; Magrakvelidze, M.; Madjet, A.; De Giovannini, U.; Castrovilli, C.; Galli, M.; Liu, C.; Månsson, E.P.; et al. Attosecond correlated electron dynamics at C60 giant plasmon resonance. *arXiv* **2021**, arXiv:2111.14464.
14. Future Directions of Quantum Information Processing: A Workshop on the Emerging Science and Technology of Quantum Computation, Communication, and Measurement. Available online: https://basicresearch.defense.gov/Portals/61/Documents/future-directions/Future_Directions_Quantum.pdf?ver=2017-09-20-003031-450 (accessed on 28 November 2023).
15. Altuntaş, E.; Spielman, I.B. Weak-measurement-induced heating in Bose-Einstein condensates. *Phys. Rev. Res.* **2023**, *5*, 023185. [CrossRef] [PubMed]
16. Escudero, R.G.; Minář, J.; Pasquiou, B.; Bennetts, S.; Schreck, F. Continuous Bose–Einstein condensation, Chun-Chia Chen. *Nature* **2022**, *606*, 683–687. [CrossRef]
17. De Motte, D.; Grounds, A.R.; Rehák, M.; Rodriguez Blanco, A.; Lekitsch, B.; Giri, G.S.; Neilinger, P.; Oelsner, G.; Il'ichev, E.; Grajcar, M.; et al. Experimental system design for the integration of trapped-ion and superconducting qubit systems. *Quantum. Inf. Process* **2016**, *15*, 5385–5414. [CrossRef] [PubMed]
18. Becher, C.; Gao, W.; Kar, S.; Marciniak, C.D.; Monz, T.; Bartholomew, J.G.; Goldner, P.; Loh, H.; Marcellina, E.; Johnson Goh, K.E.; et al. 2023 roadmap for materials for quantum technologies. *Mater. Quantum. Technol.* **2023**, *3*, 012501. [CrossRef]